Test Plan 2,4,6, Tribromophenol CAS #118-79-6

A. Physical Chemistry

Endpoint	Tribromophenol (CAS #118-79-6)
Melting point	95.5°C
Boiling point	286^{0} C
Density (relative)	2.55
Vapor pressure	5.72 x 10 ⁻⁵ mm Hg @ 25 ⁰ C
Partition coefficient (log Pow)	4.13
Water solubility	70 mg/L @ 15 ⁰ C 996 mg/L @ 35 ⁰ C
	996 mg/L @ 35 ⁰ C

Test Plan: Pertinent physical property values (melting point, boiling point, vapor pressure, n-octanol/water partition coefficient and water solubility) have been determined. No additional determinations are needed.

B. Environmental Fate and Pathways

Endpoint	Tribromophenol (CAS #118-79-6)		
Photolysis, in air (Atmospheric $T_{1/2}$)	4.6 hr		
Photolysis, in water $(T_{1/2})$	Biphasic: 1 hr, 11.5 hr		
Hydrolysis	Stable in water		
Biodegradation	Not readily biodegradable		
Distribution	Henry's Law Constant: 3.55 x 10 ⁻⁸ atm-m ³ /mole @ 25°C		
Bioaccumulation (fish)	20-fold in edible tissue		
	140-fold in viscera		

1. Photolysis

Photolysis by UV light of TBP on silica gel plates indicated a half-life of 4.6 hours.

Higher molecular weight hydrocarbon components of substances in this chemical group are predicted to have little or no tendency to partition to air. The half-life for degradation of volatilized hydrocarbons by reaction with hydroxyl radicals in the troposphere, under the influence of sunlight are predicted, by extrapolation from data quoted by Atkinson, to be less than one day.

Degradation of an aqueous solution of TBP by light from a medium pressure mercury vapor lamp was rapid and biphasic, the first phase having a half-life of about 1 hour and the second

phase of about 11.5 hours.

2. Hydrolysis

Hydrocarbons present in substances in this Group are not susceptible to hydrolysis under environmental conditions.

3. Biodegradation

Studies indicate TBP is not readily degraded by waste water bacteria when other nutrients are present. Bacteria degrade sodium TBP significantly only when there is a scarcity of other nutrients present.

4. Distribution

Henry's Law constant for TBP is 3.55 x 10⁻⁸ atm-m³/mole at 25⁰C. Actual distribution for various hydrocarbons was calculated according to Mackay Level 1 using the parameters defined in a paper by van der Zandt and van Leeuwen. Results for TBP were not included, but results for other hydrocarbons indicated that lower molecular weight alkanes and aromatic hydrocarbons partition primarily to air. With increasing distribution to soil and sediment as the molecular weight rises. (n-Tetradecane: 76.6% in air; phenanthrecene: 91.6% in soil; e-eicosane: 97.7% in soil.)

5. Bioaccumulation

The bluegill sunfish, exposed to TBP for 28 days, resulted in 20-fold bioaccumulation in edible tissue and 140-fold concentration viscera. Plateau levels were reached by 3-7 days of exposure. The half-life for residues was less than 24 hours following termination of exposure.

Test Plan: All pertinent endpoints have been satisfied. No further testing is required.

C. Aquatic Toxicity

Endpoint	Tribromophenol (CAS #118-79-6)
Toxicity to Fish	Rainbow trout: 4 day $TL_{50} = 0.24$ ppm
	Bluegill sunfish: 4 day $TL_{50} = 0.28$ ppm
Acute Toxicity to Daphnia	48 hr TL50 = 5.5 mg/L (flow-through)
Toxicity to Aquatic Plants (algae)	Not available

1. Toxicity to Freshwater Fishes

Static aquatic toxicity tests with rainbow trout and with bluegill sunfish indicated the 4 day LC50 was 0.24 and 0.28 ppm, respectively.

2. Acute Toxicity to Daphnia

A dynamic aquatic toxicity study with Daphnia magna indicated the 48 hours TL50 was 5.5ppm.

Test Plan: A test for toxicity to algae will be performed.

D. Mammalian Toxicity-Acute

Endpoint	Tribromophenol (CAS #118-79-6)		
Acute Oral	LD_{50} (rat) = 1905 mg/kg		
	LD_{50} (rat) = 3704 mg/kg		
	LD_{50} (rat) = 5012 mg/kg		
Acute Inhalation	LC ₅₀ (1 hour, rat) >200 mg/L		
	LC ₅₀ (4 hour, rat) >1.63 mg/L		
	LC ₅₀ (4 hour, rat) >50 mg/L		
Acute Dermal	LD ₅₀ (rabbit) >2000 mg/kg b.w.		
	LD ₅₀ (rabbit) >8000 mg/kg b.w.		

1. Acute Toxicity

Several studies assessed the acute oral toxicity of TBP and determined that the LD_{50} for male and female rats combined ranged from 1905 to 5012 mg/kg. Dermal LD_{50} values were reported to range from >2000 mg/kg to > 8000 mg/kg body weight.

Although TBP is not a gas at room temperature $(25^{0}C)$ an inhalation test of the dust was performed. The LC₅₀ for 1 hour exposure was >200mgL and for 4 hours exposure was >1.63 and >50 mg/L in two studies.

Test Plan: The requirements have been met. No additional testing will be performed.

E. Mammalian Toxicity-Genotoxicity

1. Genotoxicity

Tribromophenol was negative in the Ames assay in the absence and presence of metabolic activation. This test meets the requirement for gene mutation.

Test Plan: TBP has not been tested for its potential to induce chromosome aberrations *in vitro*; however, an *in vivo* chromosome aberration assay (erythrocyte micronucleus test in male and female mice), which is more relevant to predicting potential hazard to humans, was negative. No further testing is required.

F. Mammalian Toxicity-Repeated Dose/Reproduction/Developmental

Endpoint	Tribromophenol (CAS #118-79-6)		
Repeated Dose	Inhalation (3weeks), NOAEL 0.10 mg/L		
	Dermal (28 days), LOEL 100 mg/kg		
Developmental Toxicity/Teratogenicity	Inhalation, rat:		
	NOEL (developmental and developmental neurotox)		
	<0.03 mg/m ³ . NOEL (maternal and maternal neurotox)		
	$= 0.1 \text{ mg/m}^3 \text{ and } 0.3 \text{ mg/m}^3, \text{ respectively.}$		
	Gavage (pilot), rat:		
	NOEL (developmental) = 300 mg/kg/day		
	NOEL (maternal) = 300 mg/kg/day.		

1. Repeated Dose Toxicity

Rats were exposed by inhalation to dust of TBP for 6 hours/days, 5 days/week for three weeks and concentrations of 0, 0.10 and 1.00 mg/L. One male and one female died at the high dose. There were lower weight gains in the high dose males and females and in the low dose females. The NOAEL was 0.10 mg/L.

A 28 day study was conducted with rabbits exposed dermally to TBP at 100, 300, and 1000 mg/kg. The LOEL was 100 mg/kg (lowest dose tested). The treatment related effect observed was lesions in the test skin sites of all animals. No other treatment related effects were noted at 100 or 300 mg/kg. At 1000 mg/kg one animal died no other treatment related effects noted.

Test Plan: Based on the available data no further testing is necessary.

2. Development Toxicity

A Russian inhalation study in rats at levels 0.03-1.0 mg/m³ reported or LOEL of 0.3 mg/m³ for maternal toxicity and of 0.1 mg/m³ for developmental toxicity following 4 hour daily whole body inhalation exposure to TBP from day 0 of gestation through day 20 of gestation. The NOEL would be 0.1 mg/m³ for maternal toxicity and 0.03 mg/m³ for developmental toxicity.

The same group reported a inhalation developmental neurotoxicity study in rats using the same does levels as the prior study. They concluded the NOEL for developmental neurotoxicity was <0.03 mg/m³ and the NOEL for maternal neurotoxicity was 0.3 mg/m³ following 24 hour/day exposures from day 1 of gestation through day 21 gestation.

TBP was administered by gavage to rats from gestation day 6 through 15 at dose levels ranging from 10-3000 mg/kg/day. The treatment related maternal effects were slight decreases in body weights at 1000 mg/kg (NOEL for maternal effects was 300 mg/kg) and the treatment related developmental effects were slight increases in post implantation losses

and a slight decrease in the number of viable fetuses in the 1000 mg/kg/day (NEOL for developmental effects was 300 mg/kg/day).

Test Plan: Based on the available data no further testing is necessary.

3. Reproductive Toxicity

The data from the repeated dose studies showed no adverse effects on the ovaries, testis, prostrate or uterus. The data contained in the teratology and developmental neurotoxicity study showed developmental and neurotoxic effects at several dose levels. Based on the hazard information already available and the fact that tribromophenol is used as a rate limited intermediate and is incorporated into resin or plastics, it is believed that enough data already exists to assess the mammalian toxicity of the chemical. Therefore it is not necessary to fill this screening level endpoint.

Test Plan: No further testing is necessary.

Test Plan Matrix 2,4,6, Tribromophenol CAS #118-79-6

TEST ENDPOINT	Data	Data	Test
	Available	Adequate	Required
PHYSICAL CHEMISTRY			
Melting Point	Y	Y	N
Boiling Point	Y	Y	N
Vapor Pressure	Y	Y	N
n-Octanol/Water Partition Coefficient	Y	Y	N
Water Solubility	Y	Y	N
ENVIRONMENTAL FATE AND PATHWAYS			
Photodegradation	Y	Y	N
Stability in Water	S	N/A	N
Biodegradation	Y	Y	N
Transport between Environmental Compartments (Fugacity)	S	N/A	N
AQUATIC TOXICITY			
Acute Toxicity to Fish	Y	Y	N
Acute Toxicity to Daphnia	Y	Y	N
Toxicity to Aquatic Plants (algae)	N	N/A	Y
MAMMALIAN TOXICITY-ACUTE			
Acute Toxicity	Y	Y	N
MAMMALIAN TOXICITY-GENOTOXICITY			
Genetic Toxicity-Gene Mutation	Y	Y	N
Genetic Toxicity-Chromosomal Aberrations (in vivo)	Y	Y	N
MAMMALIAN TOCICITY-REPEATED			
DOSE/REPRODUCTION/DEVELOPMENTAL			
Repeated Does Toxicity	Y	Y	N
Toxicity to Reproduction	Y	Y	N
Developmental Toxicity	Y	Y	N

Y = Yes, adequate experimental data

N = No, not required

S = Data available on a similar compound

N/A = Not Applicable